The Higher Orders of the Theory of Strong Perturbations in Quantum Mechanics and the Secularity Problem

Marco Frasca

Via E. Gattamelata,3

00176 Roma (Italia)

Abstract

We solve the higher order equations of the theory of the strong perturbations in quantum mechanics given in M.Frasca, Phys. Rev. A **45**, 43 (1992), by assuming that, at the leading order, the wave function goes adiabatically. This is accomplished by deriving the unitary operator of adiabatic evolution for the leading order. In this way it is possible to show that at least one of the causes of the problem of phase-mixing, whose effect is the polynomial increase in time of the perturbation terms normally called secularities, arises from the shifts of the perturbation energy levels due to the unperturbed part of the hamiltonian. An example is given for a two-level system that, anyway, shows a secularity at second order also in the standard theory of small perturbations. The theory is applied to the quantum analog of a classical problem that can become chaotic, a particle under the effect of two waves of different amplitudes, frequencies and wave numbers.

1 Introduction

In a recent paper [1] we showed that the theory of the strong perturbations in quantum mechanics [2] gives, at the leading order, an adiabatic behavior for the quantum system which is applied to. Beside, we showed, through the interaction picture, that the validity condition $< H_0 > \ll < V >$, being the average taken on each eigenstate of the perturbation, should be verified at any time. Actually, this is a set of conditions that could give rise to secularities as we will show, being a secularity a polynomial contribution in time in the perturbation term. The secularities are normally attributed to phase-mixing in the solution of the Schrödinger equation. Actually, a resummation can be easily accomplished by comparing the result of the leading order of the strong perturbation theory with the same in the interaction picture. The only effect, however, can be a harmless shift in the energy-levels of the perturbation.

We can prove all that by deriving the unitary evolution operator for the leading order, that is, the adiabatic evolution operator for the given equation. In this way, the equations of higher orders in ref.[2] can be integrated and the above cause of secularities pointed out. This problem is exemplified through a two-level model that, however, still shows a secularity at second order.

However, it should be stressed that the model here considered suffers similar problems from the standard small perturbation theory too.

The full theory is applied to a quantum version of a well-known classical model [3], that is a particle under the effect of two waves having different amplitudes, frequencies and wave-numbers. We assume the perturbation acting from the far past, being the particle free in that limit. The model appears treatable by our method as is the one in ref.[4].

The paper is so structured. In sec.2 we derive the unitary evolution operator and the higher order equations are solved. A possible origin of secularities is given. In sec.3 we apply the theory to the case of a two-level system in a constant perturbation showing how secularities can be partially eliminated, being one of the causes the one pointed out in sec.2. In sec.4 we consider the quantized version of the classical model of the particle in interaction with two waves. In sec.5 some conclusions are drawn and the problem of the limitations of the theory is considered.

2 Higher Order Terms and Secularities

The general theory of strong pertrubations in quantum mechanics as developed in ref.[2] considers a unitary evolution operator $U(t,t_0)$ such that

$$VU(t,t_0) = i\hbar\frac{dU(t,t_0)}{dt} \tag{1}$$

being V the perturbation. The general hamiltonian of the system has the form $H = H_0 + V$ with H_0 that may also depend on time, so that a perturbation series could be derived as

$$\begin{aligned}
|\psi(t)> &= U|\psi(t_0)> \\
&- \frac{i}{\hbar}U\int_{t_0}^{t} dt' U^\dagger(t')H_0U(t')|\psi(t_0)> \\
&+ \left(-\frac{i}{\hbar}\right)^2 U\int_{t_0}^{t} dt' U^\dagger(t')H_0U(t')\int_{t_0}^{t'} dt'' U^\dagger(t'')H_0U(t'')|\psi(t_0)> \\
&+ \cdots
\end{aligned} \tag{2}$$

or, introducing the time ordering operator T, as

$$\begin{aligned}
|\psi(t)> &= U|\psi(t_0)> \\
&- \frac{i}{\hbar}U\int_{t_0}^{t} dt' U^\dagger(t')H_0U(t')|\psi(t_0)> \\
&+ \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 U\int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' T(U^\dagger(t')H_0U(t')U^\dagger(t'')H_0U(t''))|\psi(t_0)> \\
&+ \cdots
\end{aligned} \tag{3}$$

It is easy to see that the main problem is the determination of the operator U and then the computation of $U^\dagger H_0 U$ to go to higher orders. This can be easily accomplished if we consider the main results of ref.[1], that is, the leading order wave function, $|\psi^{(0)}(t)>= U|\psi(t_0)>$, is just the following adiabatic one

$$|\psi(t)>\sim \sum_n c_n e^{i\gamma_n} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' v_n(t')}|n;t> \tag{4}$$

being $c_n =< n;t_0|\psi(t_0)>$, $V|n;t>= v_n(t)|n;t>$ and

$$\gamma_n(t) = \int_{t_0}^t dt' < n;t'|i\frac{d}{dt'}|n;t'> . \tag{5}$$

This should be compared with the one obtained in the interaction picture that gives

$$|\psi(t)>\sim \sum_n c_n e^{i\gamma_n} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' <n;t'|H_0|n,t'>} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' v_n(t')}|n;t> \tag{6}$$

where level shifts appear due to the unperturbed part of the hamiltonian. We now show that these shifts could give rise to secularities for the condition $< n;t|H_0|n;t>\ll v_n(t)$.

Let us consider the evolution operator U for an adiabatic evolution. It is a simple matter to see that we can write for eq.(1)

$$U(t,t_0) = \sum_n e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' v_n(t')}|n;t>< n;t_0| \tag{7}$$

then

$$U^\dagger H_0 U = \sum_n <n;t|H_0|n;t> |n;t_0><n;t_0| + \sum_{m,n,m\neq n} e^{i[\gamma_n(t)-\gamma_m(t)]} \tag{8}$$
$$e^{-\frac{i}{\hbar}\int_{t_0}^t dt'[v_n(t')-v_m(t')]} <m;t|H_0|n;t> |m;t_0><n;t_0|.$$

We fix our attention on the first term on the rhs of the above equation. That term, when substitued in eq.(2), at the first order gives

$$-\frac{i}{\hbar}U\int_{t_0}^t dt' \sum_n <n;t'|H_0|n;t'> |n;t_0><n;t_0|\psi(t_0)> = \tag{9}$$
$$\sum_n \left(-\frac{i}{\hbar}\int_{t_0}^t dt' <n;t'|H_0|n;t'>\right) c_n e^{i\gamma_n} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' v_n(t')}|n;t>$$

from which we recognize the second term of the series development of the exponential of the level shifts in eq.(6). This term could give rise to secularities in the perturbation series if the shifts $<n;t|H_0|n;t>$ are time-independent as we are going to show in the next section. It must be noticed that the above term is a direct application of the condition $<n;t|H_0|n;t> \ll v_n(t)$ and comes directly from the theory of strong perturbations. So, as a rule, such terms should be simply resummed away. This is accomplished without difficulty by computing the level shifts and using eq.(6) as leading order. By comparing the level shifts with the energy levels of the perturbation, or if the shifts are simply harmless, we are able to realize if we can neglect such

shifts. Otherwise, we retain them and rewrite the evolution operator as

$$U(t,t_0) = \sum_n e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' <n;t'|H_0|n;t'>} e^{-\frac{i}{\hbar}\int_{t_0}^t dt' v_n(t')} |n;t><n;t_0| \tag{10}$$

redefining the full perturbation series. We will clarify the above arguments with the following example.

3 Two-Level System with a Constant Perturbation

We consider the hamiltonian

$$H = H_0 + V = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & V_{12} \\ V_{21} & 0 \end{pmatrix} \tag{11}$$

whose exact solution is well-known [5]. We apply to it the above results to exemplify the method.

The eigenstates of the perturbations are

$$|v_1> = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\frac{V_{21}}{|V_{12}|} \end{pmatrix}, |v_2> = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{V_{12}}{|V_{12}|} \\ 1 \end{pmatrix} \tag{12}$$

corresponding to the eigenvalue $-|V_{12}|$ and $|V_{12}|$ respectively. Then, we have

$$U(t) = e^{\frac{i}{\hbar}|V_{12}|t}|v_1><v_1| + e^{-\frac{i}{\hbar}|V_{12}|t}|v_2><v_2| \tag{13}$$

and

$$U^\dagger(t)H_0U(t) = \frac{E_1+E_2}{2}I + \qquad (14)$$
$$\frac{E_1-E_2}{2|V_{12}|}\left(V_{12}e^{-2\frac{i}{\hbar}|V_{12}|t}|v_1><v_2| + V_{21}e^{2\frac{i}{\hbar}|V_{12}|t}|v_2><v_1|\right)$$

being

$$<v_1|H_0|v_1>=<v_2|H_0|v_2>=\frac{E_1+E_2}{2}. \qquad (15)$$

So, the first term in the rhs of eq.(14) is just the contribution from the level shifts that, by comparing with eq.(6), reduces simply to a harmless phase factor and can be systematically neglected, the condition $|V_{12}| \gg \frac{E_1+E_2}{2}$ to be compared with the exact solution of this problem.

Our method works till second order as does the standard small perturbation theory as, at that order, a term increasing with time appears. So, we have found a possible cause of secularities but the problem is still open. However, it should be stressed that secularities are a general problem also for the standard small perturbation theory [6], the question is to understand the origin of them. This does not mean at all that the method is unuseful as we are going to show in the next section.

4 The Two-Wave Model

We consider the hamiltonian

$$H = \frac{p^2}{2m} + V_1 cos(k_1 x - \omega_1 t) + V_2 cos(k_2 x - \omega_2 t) \tag{16}$$

that can be easily quantized with the substitution $p \rightarrow -i\hbar\frac{\partial}{\partial x}$. This problem is analog to the classical one in ref.[3] of a pendulum under the effect of an oscillatory perturbation. We assume an adiabatic switching of the perturbation from $t = -\infty$, being the particle free in that limit, that is $\psi(x, -\infty) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$. This class of problems is tractable from the point of view of secularities as already shown in ref.[4] and as we are going to see in this case.

The leading order solution is then

$$\begin{aligned}\psi^{(0)}(x,t) \quad = \quad & \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} J_m\left(\frac{V_1}{\hbar\omega_1}\right) J_n\left(\frac{V_2}{\hbar\omega_2}\right) \times \\ & e^{-i(mk_1+nk_2)x} e^{i(m\omega_1+n\omega_2)t} \times \\ & \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}\end{aligned} \tag{17}$$

being J_m and J_n the Bessel functions of order m and n respectively. It is quite simple to derive

$$U^\dagger H_0 U \psi(x,-\infty) \quad = \quad \left(\frac{p^2}{2m} + \frac{k_1^2 V_1^2}{4m\hbar^2\omega_1^2} + \frac{k_2^2 V_2^2}{4m\hbar^2\omega_2^2}\right)\psi(x,-\infty) +$$

$$\sum_{\substack{m,r\\ m\neq r}}\sum_{\substack{n,s\\ n\neq s}} J_m\left(\frac{V_1}{\hbar\omega_1}\right) J_r\left(\frac{V_1}{\hbar\omega_1}\right) J_n\left(\frac{V_2}{\hbar\omega_2}\right) J_s\left(\frac{V_2}{\hbar\omega_2}\right) \times \tag{18}$$
$$\frac{(p-m\hbar k_1-n\hbar k_2)^2}{2m}\times$$
$$e^{-i[(m-r)k_1+(n-s)k_2)]x}e^{i[(m-r)\omega_1+(n-s)\omega_2)]t}\psi(x,-\infty)$$

having put $H_0=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$. It easy to see the part originating the secularities. This is the first term on the rhs that gives rise to a phase-factor due to the kinetic energy of the particle and the ponderomotive forces of the two waves. This term can be summed away. The sums in eq.(18) can be evaluated and this yields the development parameter of the perturbation series. We avoid this calculation here being not the main point of the paper, we just point out that no secularities appear at this order.

5 Conclusions

With the fundamental result of ref.[1], the theory of strong perturbations in quantum mechanics is strictly linked with the adiabatic theorem. This means that all the limitations of the adiabatic theorem should be ported to this theory. One problem may be due to a continuos spectrum of eigenvalues for the perturbation. We have avoided to face this problem in sec.4, although

meaningful results was obtained.

However, the main question remains the secularities arising from the perturbative solution of the Schrödinger equation. We are not assured that going to higher orders, secularities will not appear. We would like to stress again that this kind of problems arise normally in the standard theory of small perturbations as could be seen in ref.[6] where some methods are given to face the question.

Anyway, we showed with a lot of examples that the theory is indeed useful and a wide possibility to explore new solutions of the Schrödinger equation is surely open. This in turn means that new quantum behaviors should be considered, that is, the class of quantum systems that we define strongly perturbed.

[1] M.Frasca, "*The Leading Order of the Theory of Strong Perturbations in Quantum Mechanics*", quant-ph/9507007 (1995); M.Frasca, submitted to Nuovo Cimento (1995); see also A.Joye, Ann. Inst. Henri Poincare', **63**, 231 (1995)

[2] M.Frasca, Phys. Rev. A **45**, 43 (1992); Phys. Rev. A **47**, 2364 (1993)

[3] R.Z.Sagdeev, D.A.Usikov, G.M.Zaslavsky, *Nonlinear Physics (From the Pendulum to Turbulence and Chaos)*, Harwood Academic Publishers, Philadelphia, Penn., 1992

[4] M.Frasca, Nuovo Cimento B, **107**, 845 (1992); Nuovo Cimento B, **109**, 1227 (1994); Phys. Rev. E, **53**, 1236 (1996)

[5] J.J.Sakurai, *Modern Quantum Mechanics*, Benjamin/Cummings Publishing Company, Reading, Mass., 1985

[6] J.Kevorkian, J.D.Cole, *Perturbation Methods in Applied Mathematics*, Springer-Verlag, New York, N.Y., 1985